JOURNAL OF MOLECULAR STRUCTURE, VOLUME 240 (1990)

AUTHOR INDEX

Abu-Zeid, M.E., 225
Ando, I., 19
Ando, S., 19
Atkinson, I.M., 313

Badawi, H.M., 225
Barnes, A.J., 239
Barón, M., 31
Bator, G., 39
Bittner, A.J., 305
Blake, A.J., 95
Blom, R., 95
Butayev, B.S., 295

Caminati, W., 253, 263
Chen, X.-M., 69
Cook, M.J., 11
Cradock, S., 95

Davidson, S.L., 95
Dega-Szafran, Z., 159
Denisenko, S.N., 305
Di Bernardo, S., 253, 263

Eisenberg, C., 175
Emsley, J., 59
Engelen, B., 275
Enjalbert, R., 77
Ermakov, K.V., 295
Ewbank, J.D., 141
Exner, O., 11

Fukushima, K., 201

Galewski, Z., 39
Galy, J., 77
Grech, E., 111, 119

Hedberg, K., 151
Henning, J., 275
Howe, T.J., 11
Hrynio, A., 159

Isomura, K., 187

Jakubas, R., 39
Jones, W., 111, 119

Kamata, T., 187
Kariuki, B., 111, 119
Kasprzak, J., 127
Kasturi, A., 1
Kaupp, G., 305
Keene, F.R., 313
Kleeberg, H., 175
Konaka, S., 141
Konopka, R., 133
Krygowski, T.M., 111, 119
Krzyminiewski, R., 127, 133
Kulp-Newton, S.Q., 263
Kuroki, S., 19

Labarre, J.-F., 77
Lis, T., 47
Lutz, H.D., 275

Ma, L.Y.Y., 59
Majerz, I., 47
Mak, T.C.W., 69
Malarski, Z., 39, 47
Matuszewski, J., 39
Melnik, M., 285
Miniewicz, A., 39
Mrozinski, J., 285

Nyburg, S.C., 59

Ozaki, T., 19

Parkins, A.W., 59
Perchard, J.-P., 239
Pietrzak, J., 133
Premaswarup, D., 1
Puga, J., 89

Rademacher, P., 305
Rankin, D.W.H., 95
Ritchie, G.L.D., 331

Sabova, Z., 285
Sakurada, K., 201
Schäfer, L., 141, 263
Schriver, A., 239
Schriver, L., 239
Searle, G.H., 313
Shoji, A., 19
Siam, K., 141, 263
Singelenberg, F.A.J., 213
Sournies, F., 77
Spiridonov, V.P., 295
Szafran, M., 159
Szymaszek, A., 285

Takehara, K., 187
Takenaka, T., 187
Takeuchi, H., 141
Taniguchi, H., 187
Thomassen, H., 151

Umemura, J., 187

Van der Maas, J.H., 213
Venkatacharyulu, P., 1

Webb, G.A., 19
Wormell, P., 331
Woźniak, K., 111, 119

Yousef, Y.A., 225

Zanin, B., 77
Zanoni, R., 89
Zinn, T., 175

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 240 (1990)

SUBJECT INDEX

Acetic acids,
A quantitative comparison of spectroscopic and energy data, in solution, of NHO and OHO hydrogen bonds and gas-phase proton affinities: complexes of pyridines and pyridine *N*-oxides with acetic acids, 159
Amino hydrogen location,
Microwave spectrum and amino hydrogen location in indole, 253

Binaphthyl,
Solution-state conformation of 1,1′-binaphthyl. A Kerr and Cotton–Mouton effect study, 331
Bis (betaine) hydrochloride monohydrate,
Crystal structure of bis(betaine)hydrochloride monohydrate, 69
Bis(dimethylamino)naphthalene tetrafluoroborate,
Crystallographic studies on sterically affected chemical species. Part II. Molecular and crystal structure of 1,8-bis(dimethylamino)naphthalene tetrafluoroborate. Analysis of distortion of geometry in the aromatic part due to intramolecular hydrogen bonding, 111

Carbon tetrabromide,
Distances, root-mean-square amplitudes of vibration, and vibrational anharmonicity in carbon tetrabromide from a gas-phase electron-diffraction investigation, 151
Catechol,
Investigation of the molecular structure of catechol by combined microwave spectroscopy and ab initio calculations, 263
Chloral hydrate,
Study of γ-irradiated chloral hydrate single crystal by electron spin resonance, 127
Chloroform,
IR spectroscopic investigation of solvent effects and H-bond formation on the CD stretching frequency of chloroform, 175
Conformational equilibria,
Long-range substitutent effects on conformational equilibria, 11
$[Co\{(\pm)pn\}_n(en)_{3-n}]^{3+}$ systems,
Conformational analyses of the isomers of the $[Co\{(\pm)pn\}_n(en)_{3-n}]^{3+}$ systems: a reinvestigation (en = ethane-1,2-diamine; pn = propane-1,2-diamine, $n = 0$–3), 313
Copper(II) compounds,
Monomeric and dimeric copper(II) compounds with the 2-fluoro-6-chlorobenzoate ligand, 285
Cotton–Mouton,
Solution-state conformation of 1,1′-binaphthyl. A Kerr and Cotton–Mouton effect study, 331
trans-1,4-Cyclohexane dicarboxylic acid,
Chirality in *trans*-1,4-cyclohexane dicarboxylic acid, 31
Cyclopropylmethanol,
Conformational stability, structure and vibrational spectra of cyclopropylmethanol, 225

Diaziridines,
Orbital interactions in diaziridines, 305
2,5-Dichlorophenol,
NQR studies on 2,5-dichlorophenol, 1
Diethylene glycol diethyl ether,
Conformational change of diethylene glycol diethyl ether due to cation-capture and water-accommodation, 201
Diisopropyl sulfide,
Molecular structure and conformation of diisopropyl sulfide in the vapor phase: reinvestigation by molecular orbital constrained electron diffraction, 141
β-Diketone interactions,
β-Diketone interactions. Part 12. The structure and properties of 3-(3′,4′,5′-trimethylphenyl-pentane-2,4-dione,

$C_{14}H_{18}O_2$; the hydrogen-bond energy of the enol tautomers of β-diketones, 59
Dimethylsulphoxide–hydrogen iodide,
Infrared matrix isolation studies of dimethylsulphoxide–hydrogen iodide molecular complexes, 239
Dodecyloxyphenylpyrazine carboxylic acid,
Fourier transform-infrared spectra and molecular orientation in thin Langmuir–Blodgett films of dodecyloxyphenylpyrazine carboxylic acid and its barium salt, 187

Films,
Fourier transform-infrared spectra and molecular orientation in thin Langmuir–Blodgett films of dodecyloxyphenylpyrazine carboxylic acid and its barium salt, 187
2-Fluoro-6-chlorbenzoate ligand,
Monomeric and dimeric copper(II) compounds with the 2-fluoro-6-chlorobenzoate ligand, 285

Glycine residue,
Hydrogen-bonding effect on ^{15}N NMR chemical shifts of the glycine residue of oligopeptides in the solid state as studied by high-resolution solid-state NMR spectroscopy, 19

Hydrogen-bonding,
Fourier transform-infrared study of hydrogen-bonding between an OH-donor and a vicinal oxygen acceptor, 213
17α-Hydroxy-progesterone,
An ESR study of the stable radical in a γ-irradiated single crystal of 17α-hydroxyprogesterone, 133

Indole,
Microwave spectrum and amino hydrogen location in indole, 253
Isomers,
Conformational analyses of the isomers of the $[Co\{(\pm)pn\}_n(en)_{3-n}]^{3+}$ systems: a reinvestigation (en = ethane-1,2-diamine; pn = propane-1,2-diamine; n = 0–3), 313
Isomorphic $M(SO_3)_2 \cdot 3H_2O$,
Lattice vibration spectra. Part LVIII. OD(OH) frequency versus H-bond distance correlation diagrams: a case study for isomorphic $M(SO_3)_2 \cdot 3H_2O$ (M = Mg, Mn, Fe, Co, Ni, Zn), 275

Kerr,
Solution-state conformation of 1,1′-binaphthyl. A Kerr and Cotton–Mouton effect study, 331

Langmuir–Blodgett films,
Fourier transorm-infrared spectra and molecular orientation in thin Langmuir–Blodgett films of dodecyloxyphenylpyrazine carboxylic acid and its barium salt, 187
Lattice vibration spectra,
Lattice vibration spectra. Part LVIII. OD(OH) frequency versus H-bond distance correlation diagrams: a case study for isomorphic $M(SO_3)_2 \cdot 3H_2O$ (M = Mg, Mn, Fe, Co, Ni, Zn), 275

4-Methylpyridine,
An unusual geometrical and spectroscopic isotopic effect in the solid complex of 4-methylpyridine with pentachlorophenol, 47
Model potential functions,
Model potential functions of nonlinear XY_2 molecules, 295
Monocyclophosphazene macrocycle,
Crystal and molecular structures of the first *trans*-MACRO-ANSA monocyclophosphazene macrocycle, *trans*-$N_3P_3Cl_4[HN-(CH_2)_3-O-(CH_2)_6-O-(CH_2)_3-NH]$, 77

Nonlinear XY_2 molecules,
Model potential functions of nonlinear XY_2 molecules, 295

OH-donor,
Fourier transform-infrared study of hydrogen-bonding between an OH-donor and a vicinal oxygen acceptor, 213
Oligopeptides,
Hydrogen-bonding effect on ^{15}N NMR chemical shifts of the glycine residue of oligopeptides in the solid state as studied by high-resolution solid-state NMR spectroscopy, 19
Oxygen acceptor,
Fourier transform-infrared study of

hydrogen-bonding between an OH-donor and a vicinal oxygen acceptor, 213

Pentachlorophenol,
An unusual geometrical and spectroscopic isotopic effect in the solid complex of 4-methylpyridine with pentachlorophenol, 47

Phthalazine semi-tetrafluoroborate,
Crystallographic studies of intra- and inter-molecular interactions. Part IV. Molecular and crystal structure of phthalazine semi-tetrafluoroborate: intramolecular changes in geometry as a consequence of H-bonding, 119

Pyridines and pyridine *N*-oxide,
A quantitative comparison of spectroscopic and energy data, in solution, of NHO and OHO hydrogen bonds and gas-phase proton affinities: complexes of pyridines and pyridine *N*-oxides with acetic acids, 159

Solvent effects,
IR spectroscopic investigation of solvent effects and H-bond formation on the CD stretching frequency of chloroform, 175

Substituent effects,
Long-range substituent effects on conformational equilibria, 11

2,2,4,4-Tetramethylpentan-3-ol (TMP),
Phase transition in solid 2,2,4,4-tetramethylpentan-3-ol (TMP), 39

Tetraosmium carbonyl clusters,
Tetraosmium carbonyl clusters: an X-ray photoelectron spectroscopy (XPS) study of valence and core levels, 89

1,2,3-Trichlorobenzene,
The molecular structure of 1,2,3-trichlorobenzene determined by combined analysis of data from gas electron diffraction and liquid crystal NMR and by X-ray crystallography, 95

Trimethylphenyl-pentane-2,4-dione,
β-Diketone interactions. Part 12. The structure and properties of 3-(3′,4′,5′-trimethylphenyl)-pentane-2,4-dione, $C_{14}H_{18}O_2$; the hydrogen-bond energy of the enol tautomers of β-diketones, 59

Water accommodation,
Conformational change of diethylene glycol diethyl ether due to cation-capture and water-accommodation, 201